J. At. Mol. Sci.
doi: 10.4208/jams.052010.062610a

Vol. **1**, No. 4, pp. 318-324
November 2010

Conductance of carbon atomic wire in the environment of H_2O molecules

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Received 20 May 2010; Accepted (in revised version) 26 June 2010
Published online 2 August 2010

Abstract. The conductance of carbon atomic wire in the environment of H_2O molecules is studied by the non-equilibrium Green function method based on density functional theory. In particular, the carbon wire with seven atoms sandwiched between the Al(100) electrodes is considered. It is found that the transport properties are sensitive to the variation of the number and the position of the H_2O molecule adsorbed on the carbon wire. To our surprise, with different positions of a single H_2O molecule on the carbon wire, the equilibrium conductance shows an evident odd-even oscillatory behavior. For example, the equilibrium conductance of the carbon wire becomes bigger when the H_2O is adsorbed on the odd-numbered carbon atoms; an opposite conclusion is obtained for the H_2O adsorbed on the even-numbered carbon atoms. For the cases of two H_2O molecules, the equilibrium conductance varies largely and the contribution of the third eigenchannel becomes larger in some special configurations. The above behavior is analyzed via the charge transfer and the density of states (DOS). Reasonable explanations are presented.

PACS: 73.40.Jn. ,85.65.+h, 73.40.Gk

Key words: even-odd, equilibrium conductance, density function theory

1 Introduction

In recent years, electronic transport properties of single molecule junctions have gained tremendous interest since they may have wide variety of important applications in future electronic components such as transistors, diodes and switches [1–4]. With the advantages of experimental techniques, for example, scanning tunneling microscope and mechanically controllable break junction [5–7], measurement of current through nanoscale systems is now allowed. And a lot of interesting behaviors, such as highly nonlinear

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I-V characteristics, negative differential resistance (NDR) and electric switching behavior, are found in various systems such as organics [8], carbon nanotubes [9], DNA [10], etc. Meanwhile, considerable amounts of theoretical work have been performed to study transport properties of molecular devices [11, 12]. Among them, atomic nanowires has been an active research area for a decade in experiment and theory studies for them are the ultimate size limit of functional nanodevices. And lots of valuable and interesting results have been found from atomic wires. For example, an even-odd oscillatory conductance behavior was shown in metal [13,14], Au [15] and Pt [15] atomic wires, and also the *I-V* curves through atomic wires were strongly nonlinear. In a recent work, things were very different for the Al atomic wires [16]. For the Al atomic wires , the equilibrium conductance oscillates with a period of four atoms for wires with a typical interatomic spacing of 2.39 Å, but with another period of six atoms for the wires with the interatomic spacing of bulk fcc aluminum, 2.86 Å. A systematic study of equilibrium conductance of C and Si atomic wires was done in our recent work and some unexpected results were found [17]. Though the conductance for both of them oscillates with the number of atoms N, for the C atomic wire the conductance differences between the wires with odd number atoms and that with even number atoms becomes smaller and smaller, and saturates to a constant at last, and for the Si atomic wire, the conductance shows an even-odd oscillatory with a period of "*M*" shape.

Linear atomic chains made of carbon atoms are well known chemical species usually referred to as cumulenes. They are ideal one-dimensional molecular wires, which has long been advocated and they have been the subjects of many studies [18]. However, evidences for it are controversial and its properties are not completely known [19]. The reason may be that transport properties of a molecular devices depend not only on the characteristics of the functional molecules, but also on many other factors, for example, the contact geometry and the gate voltage. In addition, the transport properties of the system are sensitive to its surrounding environment such as the gas molecules and the H_2O molecules and in experiment this is hard to avoid. This issue has rarely been investigated theoretically, and therefore, we study the transport properties of carbon atomic wire in the environment of H_2O molecules in this paper. In particular we take the carbon wire with seven atoms sandwiched between the Al(100) electrodes as an example to find out how the transport properties change with the variation of the number and the position of the H_2O molecule on the carbon wire.

The paper is organized in the following way: the computational method and the device model are presented in Section 2. The results and discussions are given in Section 3, and a short summary is provided in Section 4.

2 Simulation model and computational method

The calculations for equilibrium conductance and Current-Voltage (*I-V*) characteristics have been performed using a recently developed first-principles package TranSIESTA-C